CHEMISTRY AND MATERIALS SCIENCE

Providing scientific excellence and leadership that meets and anticipates the needs of the Laboratory's programs

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Message from the Associate Director

In the last all hands meeting, I presented the 2004 A list for CMS. This A list was developed by the directorate's senior management team and identifies our directorate-specific goals and investment priorities for the year (see page 6). Not only does the CMS A list keenly resonate with institutional priorities, it also articulates our near-term objectives that are derivative of our four strategic themes.

Our 2004 A list continues to reiterate our fundamental principle of simultaneous excellence in science and operations. In the area of scientific excellence, we are faced with several unprecedented challenges:

Achieving the high-energy-density science capabilities requires tremendous technical and scientific breadths. CMS continues to provide excellent people and analytical resources to the NIF project, and we're planning to bring on board new experts in relevant areas

Continued on page 6 >



Corner on Science

Superheavy Elements 115 and 113 Discovered by Team of CMS and Russian Scientists

The two newest superheavy elements, 115 and 113, were recently discovered through a collaborative effort between CMS scientists from the Glenn T. Seaborg Institute, the Chemical Biology and Nuclear Science Division (CBND), and researchers from the Joint Institute for Nuclear Research (IINR) in Dubna, Russia.

The elements were produced by bombarding americium-243 targets with calcium-48 ions from the JINR U400 cyclotron (Fig. 1). The CMS Heavy Element Group, led by CBND chemist **Ken Moody**, purified the target material in November 2001 and shipped it to Russia in June 2002. The Russian scientists made the actinide targets and ran the experiment from July 14 to August 10, 2003. Independent analyses of the experimental data were then carried out in parallel by researchers at both Dubna and Livermore.

CMS postdoc **Joshua Patin** led the data analysis effort in Livermore. Each morning, Joshua downloaded the data collected in Russia the previous day and analyzed it using a program he had written in C. These analyses revealed the presence

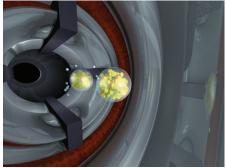


Fig. 1. An accelerated calcium-48 ion and an americium-243 target atom just before they collide. of three similar decay chains. Each chain showed five consecutive α decays over a period of about 20 seconds that terminated in a spontaneous fission of an element 105 isotope. These chains were the evidence of three separate events where a calcium nucleus had fused with an americium nucleus, creating an atom of element 115, which then decayed to element 113, and so on. Later, Joshua also found another decay chain, which showed the creation of a separate isotope of element 115.

Joshua's findings were independently verified by his Russian counterpart,

Continued on page 7 ➤

Interview With...

Alex Hamza

In March 2004, Alex Hamza was named director of the newly established Nanoscale Synthesis and Characterization Laboratory (NSCL), a joint initiative between the CMS and Engineering directorates. Alex,

who has been serving as interim director and deputy division leader for science and technology in CMS's Materials Science and Technology Division (MSTD), is responsible for managing all NSCL activities.

The NSCL was formed in response to stockpile science-and-technology needs

recently identified in the Laboratory's long-range plan. The primary mission of the NSCL is to create and exploit interdisciplinary research-and-

development opportunities in nanoscience and nanotechnology. In particular, the NSCL will focus on novel fabrication processes and

the synthesis, assembly, and atomic-scale characterization of new materials.

Alex is excited about the opportunity to establish the NSCL as a center of excellence in nanoscience and nanotechnology. Initial NSCL projects will focus on

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CHEMISTRY AND MATERIALS SCIENCE DIRECTORATE

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A PDF of this newsletter with clickable Web links can be downloaded from the CMS Web site: http://www-cms.llnl.gov/news/newsletter.html.

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Notable Publications BY MICHAEL FILLISS

On the Frontiers of Shock Physics: Opening the Door to New Science

A dream of researchers studying the dynamics of materials is to follow all aspects of a shock physics experiment. Being able to follow the materials properties changes in a dynamic event will provide new insight, not only on the behavior of materials under conditions of high strain rate, but also on the subsequent properties of the high-energy-density materials that are the goal of nuclear ignition.

Recently, **Pat Allen** of CMS CChED was asked to collaborate in interpreting the Extended X-ray Absorption Fine Structure (EXAFS) data obtained by a team from LLNL (**Bruce Remington and Steve Pollaine**) and researchers from University of Rochester, the University of Washington, and Los Alamos National Laboratory.

The experimental team reports in the March 5 issue of *Physical Review Letters* (**92**, 095504 [2004]) that EXAFS, using a laser-imploded target as a source, yields the properties of laser shocked metals on a nanosecond time scale. Specifically, the data shows that the EXAFS modulation damping in laser shocked Ti is much higher than predicted from the temperature rise alone. Pat and his colleagues explain that this was the result of the α -Ti to ω -Ti phase transformation at \sim 0.1 Mbar.

This work is an early and important success in applying modern materials spectroscopic tools—tools with atomic resolution—to the challenging research environment of materials dynamics and multi-phase equation of state research.

Publication URL:

http://link.aps.org/abstract/PRL/v92/e095504/

Water, Water, Everywhere ...

There are so many ideas, concepts, and materials that we take for granted but do not understand. Among these is water. However, that is changing and our knowledge is expanding because of experimental and theoretical efforts. CChED's I-Feng W. Kuo and Christopher J. Mundy are helping to create new insight into an old but unsolved problem, the aqueous liquid-vapor interface.

By applying molecular dynamics (MD) to a "stabilized" region of bulk water in the center of a water slab, they were able to quantify the various surface moieties and the surface relaxation. Their calculations are published in the January issue of *Science* (303, 658 [2004]).

The accompanying figure is a representation of the theoretical picture that resulted from their computations. In an introductory article in the same issue of *Science* magazine (303, 634, [2004]), Dominik Marx notes that the computations are not unlike throwing tetrahedral dice (the water molecules on the surface). He praises their pioneering work by noting, "The pioneering study



Snapshot of the calculated aqueous liquid-vapor interface. The individual water monomers are represented by yellow cylinders. The colored isosurfaces on the top represent the HOMO. whereas the colored isosurfaces at the bottom represent the LUMO. The orbitals are obtained by direct diagonalization of the KS matrix, indicating that the reactivity of the water slab is localized on the surface for protons and electrons

by Kuo and Mundy demonstrates that such mesoscopic phenomena will soon be studied routinely, combining both realistic modeling and first-principles simulation. Thus, ab initio molecular dynamics has a bright future!"

Publication URLs:

http://www.sciencemag.org/cgi/reprint/303/5658/658.pdf and http://www.sciencemag.org/cgi/reprint/303/5658/634.pdf ■

Please send items for the next newsletter (e.g., directorate news, awards, conference calendar items) to **Stephanie Shang** (shang2@llnl.gov). April 2004

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Directorate News

Developing the Leaders Among Us

Leadership development is an integral part of the strategic planning process for Chemistry and Materials Science. In March, CMS launched a new 12-month leadership development program with the intent of accelerating the pace at which individuals are prepared to fill leadership roles at all levels.

The program objectives are to:

- Build a diverse set of future leaders
- Accelerate development of leaders at all levels
- Enhance our program/project management skills
- Broaden our model for scientific leaders, coupling strong S&T record of accomplishment with managerial skills and leadership competencies
- Increase succession planning
- Emphasize the building and development of emotional intelligence

The program has identified three levels of leadership, each with specific development needs and methods.

Emerging: This will be targeted at individuals who are probably not in "formal" leadership roles at this time but are showing high potential. The CMS emerging leadership development program will be launched in the future.

Developing: Intended for individuals who are currently in "formal" leadership assignments such as program element leader or scientific capability leader and developing in areas where experience and coaching are needed. The CMS leadership development program was launched to focus on individuals at this level.

Executive: Targeted at individuals who are in formal, high-level leadership roles, having significant impact on others. CMS Associate Director Tomás Díaz de la Rubia is leading the succession management in this area.

Individuals have already been nominated for this initial leadership development program by the division leaders, materials program leaders, deputy associate directors, and operations managers and were then selected by CMS senior managers. Participants were chosen based on defined criteria, which included:

- Track record of proven performance, with scientific/technical breadth
- Some leadership experience as a team or project leader or in other leadership capacities
- Demonstrated ability to guide others toward given results
- Exhibit initiative and proactive approaches to problem-solving and



continually improving work processes and outcomes

- Ability to communicate effectively orally and in writing
- Observed willingness to work on one's own development, inside or outside the Laboratory
- Demonstrated commitment to LLNL and its mission

The CMS program is using a combination of coursework taught by leading management practitioners and consultants along with discussions involving leaders from LLNL, UC, and NNSA. Consultants from the Human Resources' Employee and Organizational Development Division (EODD) are assisting in program coordination and oversight. The majority of the program will be presented at or near the Laboratory.

If you'd like to learn more about the program, please contact your division leader or operations manager.

Parking in the "Back Forty" ... A Perfect Time to Start Your New Exercise Plan!

Let's face it. Sometimes finding a parking spot at the Lab can be a bit of a pain, especially with the assorted construction projects under way. The construction of Building 242, just north of Building 235, is starting to make it more challenging for CMS employees who travel to Building 235 in their personal vehicles.

If you're attending a meeting in Building 235, be sure to allow yourself enough time to park and walk from the parking lot.

It might also help to keep in mind that a little exercise is good for you!

Here are some parking lot options to consider when you're heading toward Building 235:

- Parking Lot B-4, east of Building 241, is limited.
- Parking Lot C-4, north of Building 341, is open.
- Parking Lot C-5W, north of West Inner Loop Drive, is open. ■

Tom Tombrello ... Thank You!

Professor Thomas Tombrello, Jr.—chair of the Physics, Mathematics, and Astronomy Division at California Institute of Technology—has been chairman of the CMS Directorate Review Committee since 1986. During this time, he has provided invaluable advice and assistance aimed at strengthening the quality of our staff and scientific efforts. He has been a true friend of our directorate and LLNL.

Dr. John Poate, chief technology officer and vice president for Axcelis Technologies, Inc., has agreed to take over responsibility as chairman after the next DRC meeting, scheduled for May 5–7.

We greatly appreciate Prof.

Tombrello's assistance and welcome

Dr. Poate as the new chairman.



Awards and Personnel News

CMS Scientists Honored for Scientific Achievements and Leadership

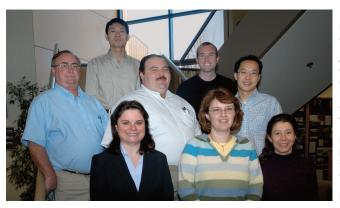
- Bryan Balazs, a CMS group leader, has been selected to receive the 2004 Petersen Award from the California Section of the American Chemical Society (ACS). The Petersen Award, presented each year at the section's annual awards meeting, recognizes a section member with the most cumulative service to the local group. The event is scheduled for Saturday, May 22, 11 a.m.–2 p.m. at Hs Lordships Restaurant at the Berkeley marina. Bryan, who is currently a California Section member-at-large, was also elected to the ACS Committee on Education for 2004–2006. This committee ensures that ACS educational activities focus on critical chemical education issues across all levels of instruction.
- Ken Moody, staff scientist in the Stockpile Radiochemistry Group, was recently given an Environmental Protection Department (EPD) directorate award. Ellen Raber, EPD department head, and Al diSabatino, facility manager for Bldg. 251, presented the award. Ken assisted EPD during its inventory reduction project in Bldg. 251 and answered technical questions posed by the EPD staff about some radioactive material that had been stored below ground there. He also supplied the staff with the names of individuals who would potentially take the "more exotic" materials left in the facility.
- Dick Quigley, a CMS excess acquisitions coordinator, will start his four-year term on the Board of Directors of the Alameda County Flood Control and Water Conservation District. Zone 7 Water Agency—short for Alameda County Flood Control and Water Conservation District—is responsible for providing flood control and water resources to the Livermore–Amador Valley. Of Alameda County's 10 active zones, only Zone 7 has its own elected seven-member board of directors. As the Tri-Valley's water "wholesaler," Zone 7 sells treated water primarily to four retail water agencies: the

- California Water Service Company, the cities of Livermore and Pleasanton, and the Dublin San Ramon Services District. It also sells untreated water directly to agricultural and other customers.
- The Minerals, Metal, and Materials Society (TMS) has awarded **Andrea Hodge**, a CMS postdoc, the TMS Young Leader Internship Award. Given annually by the Structural Materials Division of the TMS, the Young Leader Award recognizes leadership potential in young scientists and provides an honorarium as well as travel and lodging for the TMS annual meetings. Andrea's current research focuses on developing nanostructured metal foams for high-energy-density experimental targets. A profile of Andrea and her work is available in the January 2004 issue of the *CMS Directorate News*. http://www-cms.llnl.gov/news/newsletter.html
- The Materials Information Society, ASM International, has selected **Patrice Turchi**, a CMS physicist, to serve on the Alloy Phase Diagram Committee. The charter of ASM is to develop and improve publications and services that benefit the worldwide materials community.
- CMS 2002 Annual Report received an Award of Excellence from the Southern Arizona Chapter of the Society of Technical Communication (STC). In addition to highlights and accomplishments by more than 30 authors, a team including Mike Fluss, Theresa Healy, Dabbie Bowron, Emmeline Chen,

Missy Davidson, and **Scott Dougherty** contributed to the high-quality debut of the annual report. The complete report may be downloaded from the CMS Web site: http://www-cms.llnl.gov/news/ann_rpt.html ■



The Directorate warmly welcomes seven new employees and four postdocs who joined the organization over the past few months.



From left, top row: MSTD postdocs Morris Wang and Jeremy Gray. Middle row: MSTD engineer James McNeese, MSTD technician Jessee Welch, CBN chemist Jeff Tok Bottom row: OPS associate administrator Barbara Jackson, MSTD postdoc Raluca Negres, and CBN postdoc Julie Smith, Not pictured: CBN engineer Sandra Anderson, CBN administrative assistant Eryn Davis, and CBN physicist Young Ham.

So Long, Farewell, Good-Bye...

CMS would like to thank the following employees as they move on to other areas within the Laboratory:

Paul Sandoval, MSTD scientific associate

Kathleen Tarlow, AD staff administrative assistant ■



Making Us Proud: CMS Recipients of Directorate Awards

Exceptional

Joshua Patin, Ken Moody, John Wild, Mark Stoyer, Nancy Stoyer, Dawn Shaughnessy, Jackie Kenneally, and Ron Lougheed, discovery of the transactinide elements 113 and 115

David Eaglesham, elected Vice President and President elect of the Materials Research Society

John Elmer, elected as a Fellow of the American Society for Metals International Society

Christian Mailhiot, elected an American Physical Society Fellow in the Division of Materials Physics

Excellence

Ken Moody and **John Wild**, recognition of your many contributions to advance heavy element and superheavy element science at LLNL to a position of international prominence

Excellence in Publication

Chris Mundy and **I-Feng W. Kuo**, "An ab initio molecular dynamics study of the aqueous liquid-vapor interface"

Stavros Demos, Harry Radousky, Christopher W. Carr, Alexander M. Rubenchik, and Michael D. Feit, contributions to a series of three outstanding papers in the area of laser damage in optical materials published in the *Physical Review Letters* within a period of nine months



From left: Joshua Patin, Dawn Shaughnessy, Jackie Kenneally, John Wild, Ken Moody, Stavros Demos, Bryan Reed, Rebecca Browning, Kevin Moore, Adam Schwartz, Alex Hamza, Harry Radousky, Tomás Díaz de la Rubia, Mark Wall, Michael Feit, Geoff Campbell, Wayne King

Distinguished

Bryan Balazs, receiving the 2004 Petersen Award from the California Section of American Chemical Society

Vasily Bulatov, organizing the 2nd International Workshop "Multiscale Modeling of Strength and Fracture: Linking through the Mesoscale" Berkeley, CA, January 7–9, 2004

Doug Higby, effort during the seismic upgrade and moving CMS personnel into Building 155

Roseanne Kamerdula, moving and protecting the integrity of the stockpile radiochemistry vaults

Randy Simpson, organizing and chairing the Synthesis, Characterization, and Properties of Energetic/Reactive Nanomaterials Series at the Materials Research Society Conference in 2003

Jim Tobin, organizing the highly successful and inaugural Actinides Symposium held at the Materials Research Society Symposium Boston, MA, December 1–5, 2003

Wayne King, Geoff Campbell, Mukul Kumar, Alex Hamza, Kevin Moore, Adam Schwartz, Mark Wall, John Bradley, Dave Eaglesham, Alexander Ziegler, Rebecca Browning, and Bryan Reed, organizing the 9th International Conference on Frontiers of Electron Microscopy in Materials Science Berkeley, CA, October 5–10, 2003 ■



From left: Roseanne Kamerdula, Jim Tobin, Doug Higby, Bryan Balazs, David Eaglesham, Tomás Díaz de la Rubia, Christian Mailhiot, Randy Simpson, Chris Mundy, Elaine Chandler, Rich Couch, Robert Rudd

Patent Award

Alan F. Jankowski (MSTD), Jeffrey D. Morse (EE-EETD) MEMS-Based Thin-Film Fuel Cells, U.S. Patent 6,638,654 B2 October 28, 2003

A microelectromechanical systems— (MEMS-) based thin-film fuel cell for electrical power applications. The MEMS-based fuel cell may be of a solid-oxide type, a solid-polymer type, or a proton-exchange-membrane type. Each

fuel cell basically consists of an anode and a cathode separated by an electrolyte layer. In addition, catalyst layers can separate the electrodes (cathode and anode) from the electrolyte. Gas manifolds are used to transport the fuel and oxidant into each cell and to provide a path for exhaust gases. The electrical current generated from each cell is drawn away by an interconnect and support structure integrated with the gas manifold. The

fuel cells use integrated resistive heaters for efficient heating of the materials. By combining MEMS technology with thin-film deposition technology, thin-film fuel cells with microflow channels and fully integrated circuitry can be produced. These fuel cells will lower operating temperatures of the electrical power application and will yield an order-of-magnitude greater power density than currently known fuel cells. ■



Message from the Associate Director Continued from page 1

for the future. In addition, CMS has launched the Nanoscale Synthesis and Characterization Laboratory in partnership with Engineering. Its ambitious goals include the development of technology that leads to new novel materials and complex assemblies for inertial confinment fusion and high-energy-density experiments. In 2004, the NSCL has already gathered significant momentum, and an ambitious strategic initiative on double-shell ignition targets is in the planning stages. We are also making technology investments aimed at bringing to the laboratory advanced technologies that may lead to novel target materials in the future.

CMS scientists continue to make tremendous progress in the enhanced surveillance campaign, and while challenges remain daunting for 2004, we anticipate continued success in this area. To realize the capabilities in ultrafast, dynamic diagnostics, we have acquired in 2004 a new transmission electron microscope and we're building an ultrafast electron diffraction instrument to study complex transient phenomena with unmatched spatial and temporal resolution. This work is also sponsored by an LDRD Strategic Initiative in 2004 in collaboration with scientists in DNT, NIF, and PAT.

Our investments in chemical biology and bioanalytical sciences are starting to pay off big time, both in terms of outstanding scientific publications as well as in terms of our ability to capitalize on new opportunities in areas of biosecurity. For 2004, we expect to continue making investments in this area, and to align our activities to optimize the Lab's position in the DOE's Genomiscs:GTL program as well as within emerging areas in biomolecular materials in the Office of Basic Energy Sciences.

High-performance computing continues to be a crosscutting theme. With the promise of hundreds of thousands of processors and the unprecedented peak speed of Thunder and BlueGene/L, we are on the warpath to petaFlop/s within the next few years. As one of the leaders in the utilization of largescale computing, CMS users are in a strong position to continue the many scientific breakthroughs in wide-ranging applications.

In the area of operation excellence, we are firmly committed to continued implementation of the Institutional Pay and Performance Program. In 2004, we anticipate new processes for the 100, 400, and 500 series.

We have begun the first CMS Leadership Development Program in March. Launched in March 2004, this program is aimed at what we have termed "developing leaders." Future programs will be expanded to include emerging leaders as well.

Of all the priorities we have defined for 2004, none is more important than safety and security. After several years of improvement in our ES&H indexes, we are seeing an alarming reversal. While the most recent data are improving, we need to do better. Personal accountability remains the best safeguard against potential hazards.

The CMS A list will be our guide this year as we allocate resources and prioritize our responsibilities.

The List

- Continue supporting NIF construction and craft long-term effort in advanced optical materials in partnership with NIF
- Continue to lead and execute materials science and chemistry efforts to determine pit lifetimes, and develop and execute robust plans for new programs in materials science R&D of strongly driven systems for HED, ICF, and JASPER targets and impactors
- Successfully execute rad/nuc countermeasures, forensics, and nuclear attribution efforts in support of nonproliferation and homeland security programs
- Partner with BBRP to develop strategy for the Genomics:GTL Program and obtain early funding, and couple Lab-wide chem/bio/materials research efforts to longrange biosecurity plans in NAI/HSO



- Support the Yucca Mountain effort with corrosion and metallurgy expertise, while at the same time helping E&E develop new programs in water, climate modeling and hydrogen production
- Provide leadership in LLNL path forward to petaFlop-class highperformance scientific computing applications, including new science on Thunder and BlueGene/L platforms
- Realign DOE/OBES programs along CMS strategic plan and increase level of funding by \$1M/year
- Execute a successful transition to e-IWS and ITS systems, and ensure that CMS continues to operate safely within a secure and fiscally sound environment
- Implement and successfully execute the first CMS Leadership Development Program for developing leaders
- Ensure a fair IPPP process with strong coupling between performance appraisal, total contribution, ranking, and pay

Conference Calendar

DATE	CONFERENCE	LOCATION	WEB SITE
May 17–21, 2004	AUG, CGU, SEG, EEGS 2004 Joint Assembly	Montreal, Canada	http://www.agu.org/meetings/sm04/
June 20–25, 2004	Gordon Research Conference on Energetic Materials	Tilton, NH	http://www.grc.uri.edu/programs/ 2004/enermat.htm
July 4–9, 2004	Gordon Research Conference on Computational Chemistry	Plymouth, NH	http://www.grc.uri.edu/programs/ 2004/compchem.htm
September 5–10, 2004	Fourteenth International Conference on Ion Beam Modification of Materials	Monterey, CA	http://www2.avs.org/chapters/ nccavs/ibmm/

April 2004

dramistry materials science

Corner on Science Continued from page 1

Vladimir Utyonkov. The team then submitted a paper about their discovery to *Physical Review C* in September 2003. The journal article was published in February 2004, as was a front-page article about the new elements in the *New York Times*.

The discovery of these new superheavy elements proves long-held nuclear theories regarding the ultimate limits of the periodic table of the elements and the existence of the "island of stability," a predicted region of isotopes of the superheavy elements with half-lives that are longer by several orders of magnitude than the half-lives of other superheavyelement isotopes.

The element discovery also helps scientists to better understand how nuclei are held together and how they resist the fission process. The skills honed by conducting these heavy-element experiments can then be applied to solving national needs like stockpile stewardship and homeland security. For example, an improved understanding of the fission process will enable scientists to enhance the safety and reliability of the nation's nuclear stockpile and nuclear reactors.

The joint Russian–Livermore team

is now embarking on experiments to create element 112 by bombarding uranium-238 targets with calcium-48 ions. Future experiments are also being planned that will explore the chemical properties of the newly discovered superheavy elements.

CMS congratulates Ken, Joshua, and the other members of the Heavy Element Group (Fig. 2)—John Wild, Mark Stoyer, Nancy Stoyer,

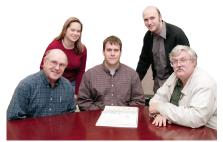


Fig. 2. Members of the CMS Heavy Elements Group in January 2004 (I–r): Jerry Landrum (retired), Dawn Shaughnessy, Joshua Patin, Philip Wilk, and Ken Moody. Not pictured: John Wild, Mark Stoyer, Nancy Stoyer, Jackie Kenneally, and Ron Lougheed (retired).

Jackie Kenneally, Ron Lougheed (retired), Jerry Landrum (retired), Philip Wilk, and Dawn Shaugnessy—for their groundbreaking scientific achievement. The increased insights into the nature of nuclear stability will impact many related scientific and technological areas.

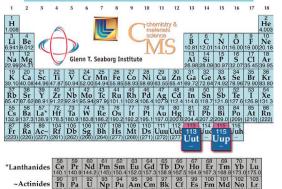
For More Information...

Visit the CMS Web site at http://www-cms.llnl.gov/e113_115/.

Related Publication

Oganessian, Y. T. et al. Experiments on the synthesis of element 115 in the reaction ²⁴³Am(⁴⁸Ca, xn)^{291-x}115. *Phys. Rev.* C **69**, 021601 (2004). Available at http://link.aps.org/abstract/PRC/v69/e021601. ■





Interview With... Continued from page 1

solving materials issues for high-energy-density targets used in the National Ignition Facility and other stockpile stewardship experimental platforms. These projects will explore nanocrystalline and nanoporous materials. Future research will address nonproliferation and other national-security issues and will expand into all areas of nanomaterials science.

The partnership with Engineering will yield valuable contributions to microassembly and precision fabrication issues. Alex looks forward to working closely with a deputy leader from Engineering and is enthusiastic about the NSCL team members that have been selected thus far: senior staff members Joe Satcher, Troy Barbee, Mike McElfresh, and Alan Jankowski from CMS and Keith Carlisle and Harry Martz from Engineering; CMS postdocs Andrea Hodge, Sergei Kucheyev, and Morris Wang; and MSTD physicist Juergen Biener.

Several collaborations between the NSCL and researchers at universities (**Jonah Erlebacher** at Johns Hopkins University and **Stephanie Brock** at Wayne State University) and other national laboratories (**Mike Pellin** at Argonne National Laboratory) have been established, and additional partnerships with academic research centers are expected. These collabora-

tions will ensure that the NSCL remains at the leading edge of new breakthroughs in nanomaterials science.

After graduating from the Massachusetts Institute of Technology in 1981 with undergraduate and master's degrees in chemical engineering, Alex attended Stanford University and received a Ph.D. in chemical engineering in 1986. As an Alexander von Humboldt fellow at the Fritz Haber Institute in Berlin, Alex continued his work with molecular-beam scattering on solid surfaces and began conducting laser—surface interaction studies. He then accepted a postdoctoral position at Sandia National Laboratories, Livermore, where he used two-photon photoemission techniques and electron-stimulated desorption to examine the properties of diamond surfaces.

Alex's career at the Laboratory began in the fall of 1989. As a chemical engineer in the Laser Interactions Group, Alex investigated laser damage issues by studying interactions between lasers and optical materials. He also explored surface characterization techniques and examined the interactions of buckyballs and highly charged ions with various surfaces. In 1999, Alex moved into CMS management as the group leader for Surface Science. He was named the group's scientific capability leader in 2000 and became MSTD's deputy division leader for science and technology in the fall of 2001.



Postdoc News





Three days after graduating from the Massachusetts Institute of Technology (MIT) with his Ph.D. in nuclear engineering, **Wei Cai** arrived at the Laboratory and started his postdoctoral career as a Lawrence fellow, working primarily in CMS's Materials Science and Technology Division as a member of the High-Performance Computational Materials Science and Chemistry Group.

Wei was initially introduced to Livermore when he joined his MIT research advisor **Sidney Yip**, a member of CMS's Directorate Review Committee, on a Laboratory-sponsored project investigating the use of theoretical models and computer simulations to understand and predict material properties. Another research mentor, **Vasily Bulatov**, directed Wei's research and taught him about simulations and dislocation dynamics for two years before leaving MIT to join CMS. Vasily later referred Wei to the Lawrence

Postdoc People News

Recent alumni of the CMS
 Postdoctoral Program include Tony
 Esposito, Brad Hart, and Tina
 Jayaweera. We wish them the best.

Fellowship Program and has mentored Wei throughout his fellowship.

The Lawrence Fellowship has provided Wei with tremendous research flexibility. Wei's primary project, helping to develop a massively parallel code for modeling dislocation dynamics, builds upon his dissertation work—computer simulations of the effect of atomistic-scale defects on material properties. Wei has also collaborated with Giulia Galli, leader of the Quantum Simulations Group in the Physics and Advanced Technologies Directorate, to model magnetic-field effects on the electronic structure of materials. In addition, Wei has enjoyed fruitful discussions with Malvin Kalos, a Defense and Nuclear Technologies Directorate scientist hailed as the father of quantum Monte Carlo simulations. Wei is now applying Malvin's importance sampling methods in an attempt to extend the time scale of large atomistic simulations.

Wei has enjoyed his many collaborations with Livermore scientists and appreciates the Laboratory's dynamic environment that makes such partnerships possible. He also values the friendships he has made in CMS, particularly with the other postdocs and scientists in his group. Wei sums up his postdoctoral experience as fun, productive, and filled with positive interactions.

Postdoc News

Congratulations to Roger Qiu for his cover article titled "Molecular modulation of calcium oxalate crystallization by osteopo-



nin and citrate," published in the February 17 issue of the *Proceedings* of the National Academy of Sciences (101, 1811 [2004]). Publication URL: http://www.pnas.org/cgi/reprint/101/7/1811.pdf

Professor Richard Reis of Stanford University, author of Tomorrow's Professor: Preparing for Academic Careers in Science and Engineering, was guest

TOMORROW'S
PROFESSOR
Preparing For
Academic Careers in
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Postdoctoral
Acceptable held

speaker at the CMS Postdoctoral Program quarterly meeting held on February 25. Dr. Reis spoke on a subject relevant to many postdocs: "From Postdoctoral Scholar to University Professor: And the Strategies You Need to Get There." His listsery, called Tomorrow's Professor, offers the latest ideas and practices in higher education, insights on how to prepare for academic careers, ways to improve teaching and learning, and suggests strategies for optimizing academic career success. If you're interested in subscribing to the e-mail service, visit http://sll.stanford.edu/ projects/tomprof/newtomprof/ subscribe.html.

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